Supplemetary Materials

Preparation of 1,3,5-tris(bromomethyl)-2,4,6-trimethylbenzene

To a mixture of mesitylene (12.0 g; 0.10 mol), paraformaldehyde (10.0 g; 0.33 mol), and 50 mL of glacial acetic acid was added 20 mL of a 31 wt% HBr/acetic acid solution rapidly. The mixture was kept for 12 h at 368 K and then poured into 500 mL of water. The product was filtered off on a G3 glass frit and dried in vacuum. The yield was 36.3 g (91 %) of l,3,5-tris(bromomethyl)-2,4,6-trimethylbenzene as a white powder.

Preparation of 1,3,5-Tri(triazol-1-ylmethyl)-2,4,6-trimethylbenzene (tttmb)

Triazole (2.76 g, 40 mmol) was dissolved in dry acetonitrile (50 mL), and anhydrous potassium carbonate (10 g) was added to the above solution. After 2 h of stirring, 1,3,5-tris(bromomethyl)-2,4,6-trimethylbenzene (4.0 g, 10 mmol) was added. The mixture was then vigorously stirred and refluxed for 12 h at 353 K. A white residue was obtained after filtering and evaporating the filtrate in a vacuum. The crude product was recrystallized from water and then ethanol/hexane (1:1) to give white crystalline product. Yield: 82%.

Table S1. Selected bond lengths /Å and angles /°for **1-3.**

Complex 1			
N(7)-Cd(1)#1	2.338(8)	N(3)-Cd(1)#2	2.307(9)
O(3)-Cd(1)#3	2.460(7)	O(4)-Cd(1)#3	2.412(8)
N(4)-Cd(1)	2.349(9)	O(1)-Cd(1)	2.459(7)
O(2)-Cd(1)	2.452(7)	Cd(1)-N(3)#4	2.307(9)
Cd(1)-N(7)#5	2.338(8)	Cd(1)-O(4)#6	2.412(8)
Cd(1)-O(3)#6	2.460(7)	N(3)#4-Cd(1)-N(7)#5	178.0(4)
N(3)#4-Cd(1)-N(4)	93.4(4)	N(7)#5-Cd(1)-N(4)	84.6(4)
N(3)#4-Cd(1)-O(4)#6	86.5(3)	N(7)#5-Cd(1)-O(4)#6	92.9(3)
N(4)-Cd(1)-O(4)#6	84.4(3)	N(3)#4-Cd(1)-O(2)	93.4(3)
N(7)#5-Cd(1)-O(2)	86.8(3)	N(4)-Cd(1)-O(2)	84.5(3)
O(4)#6-Cd(1)-O(2)	168.9(3)	N(3)#4-Cd(1)-O(3)#6	92.1(4)
N(7)#5-Cd(1)-O(3)#6	89.2(3)	N(4)-Cd(1)-O(3)#6	136.8(3)
O(4)#6-Cd(1)-O(3)#6	53.1(2)	O(2)-Cd(1)-O(3)#6	137.9(3)
N(3)#4-Cd(1)-O(1)	87.1(3)	N(7)#5-Cd(1)-O(1)	94.7(3)
N(4)-Cd(1)-O(1)	136.8(3)	O(4)#6-Cd(1)-O(1)	138.5(2)
O(2)-Cd(1)-O(1)	52.5(2)	O(3)#6-Cd(1)-O(1)	86.2(2)
Complex **2**			
Cd(1)-N(5)#1	2.288(5)	Cd(1)-N(1)	2.318(5)
Cd(1)-O(5)	2.346(5)	Cd(1)-O(4)#2	2.354(5)
Cd(1)-O(2)	2.370(6)	Cd(1)-O(1)	2.471(5)
Cd(1)-O(3)#2	2.570(5)	N(5)-Cd(1)#3	2.288(5)
O(3)-Cd(1)#4	2.570(5)	O(4)-Cd(1)#4	2.354(5)
N(5)#1-Cd(1)-N(1)	168.69(19)	N(5)#1-Cd(1)-O(5)	86.40(19)
N(1)-Cd(1)-O(5)	84.8(2)	N(5)#1-Cd(1)-O(4)#2	91.3(2)
N(1)-Cd(1)-O(4)#2	90.0(2)	O(5)-Cd(1)-O(4)#2	135.4(2)
N(5)#1-Cd(1)-O(2)	94.0(2)	N(1)-Cd(1)-O(2)	97.3(2)
O(5)-Cd(1)-O(2)	143.0(2)	O(4)#2-Cd(1)-O(2)	81.6(2)
N(5)#1-Cd(1)-O(1)	94.3(2)	N(1)-Cd(1)-O(1)	92.9(2)
O(5)-Cd(1)-O(1)	91.1(2)	O(4)#2-Cd(1)-O(1)	133.43(18)
O(2)-Cd(1)-O(1)	51.9(2)	N(5)#1-Cd(1)-O(3)#2	83.96(18)
N(1)-Cd(1)-O(3)#2	87.89(19)	O(5)-Cd(1)-O(3)#2	82.6(2)

O(4)#2-Cd(1)-O(3)#2	52.89(17)	O(2)-Cd(1)-O(3)#2	134.3(2)
O(1)-Cd(1)-O(3)#2	173.59(19)		
Complex **3**			
N(6)-Cd(1)#1	2.305(5)	N(9)-Cd(1)#2	2.377(5)
O(4)-Cd(1)#3	2.396(5)	O(3)-Cd(1)#3	2.424(6)
Cd(1)-N(6)#4	2.305(5)	Cd(1)-O(2)	2.304(5)
Cd(1)-N(1)	2.340(5)	Cd(1)-N(9)#5	2.377(5)
Cd(1)-O(4)#6	2.396(5)	Cd(1)-O(3)#6	2.424(6)
Cd(1)-O(1)	2.595(5)	N(6)#4-Cd(1)-O(2)	130.09(17)
N(6)#4-Cd(1)-N(1)	94.6(2)	O(2)-Cd(1)-N(1)	85.40(19)
N(6)#4-Cd(1)-N(9)#5	92.08(19)	O(2)-Cd(1)-N(9)#5	87.35(19)
N(1)-Cd(1)-N(9)#5	172.28(18)	N(6)#4-Cd(1)-O(4)#6	83.28(19)
O(2)-Cd(1)-O(4)#6	146.12(17)	N(1)-Cd(1)-O(4)#6	99.12(19)
N(9)#5-Cd(1)-O(4)#6	85.5(2)	N(6)#4-Cd(1)-O(3)#6	136.05(19)
O(2)-Cd(1)-O(3)#6	93.83(18)	N(1)-Cd(1)-O(3)#6	86.37(18)
N(9)#5-Cd(1)-O(3)#6	91.47(19)	O(4)#6-Cd(1)-O(3)#6	53.39(18)
N(6)#4-Cd(1)-O(1)	77.63(17)	O(2)-Cd(1)-O(1)	52.47(15)
N(1)-Cd(1)-O(1)	90.06(17)	N(9)#5-Cd(1)-O(1)	87.62(17)
O(4)#6-Cd(1)-O(1)	159.43(17)	O(3)#6-Cd(1)-O(1)	146.30(17)

Symmetry transformations used to generate equivalent atoms in (**1**): #1 − x, y − 1/2, −z + 3/2; #2 x − 1/2, −y + 3/2, −z + 2; #3 x + 1/2, −y + 5/2, −z + 2; #4 x + 1/2, −y + 3/2, −z + 2; #5 −x, y + 1/2, −z + 3/2; #6 x − 1/2, −y + 5/2, −z + 2; (**2**): #1 x + 1/2, −y + 1/2, z + 1/2; #2 −x + 3/2, y + 1/2, −z + 3/2; #3 x − 1/2, −y + 1/2, z − 1/2; #4 −x + 3/2, y − 1/2, −z + 3/2; (**3**): #1 x, −y + 1, z + 1/2; #2 x + 1/2, −y + 1/2, z + 1/2; #3 −x + 3/2, y + 1/2, −z − 1/2; #4 x, −y + 1, z − 1/2; #5 x − 1/2, −y + 1/2, z − 1/2; #6 −x + 3/2, y − 1/2, −z − 1/2.
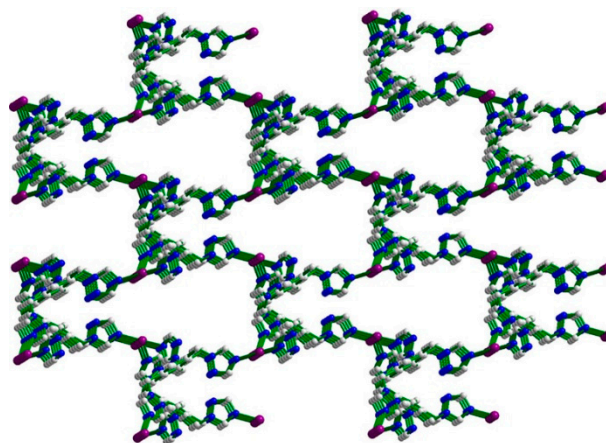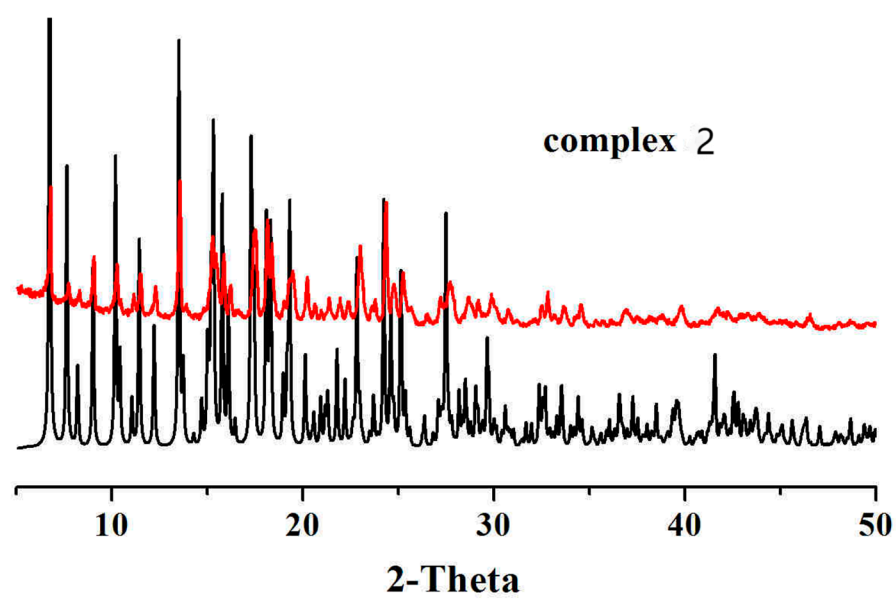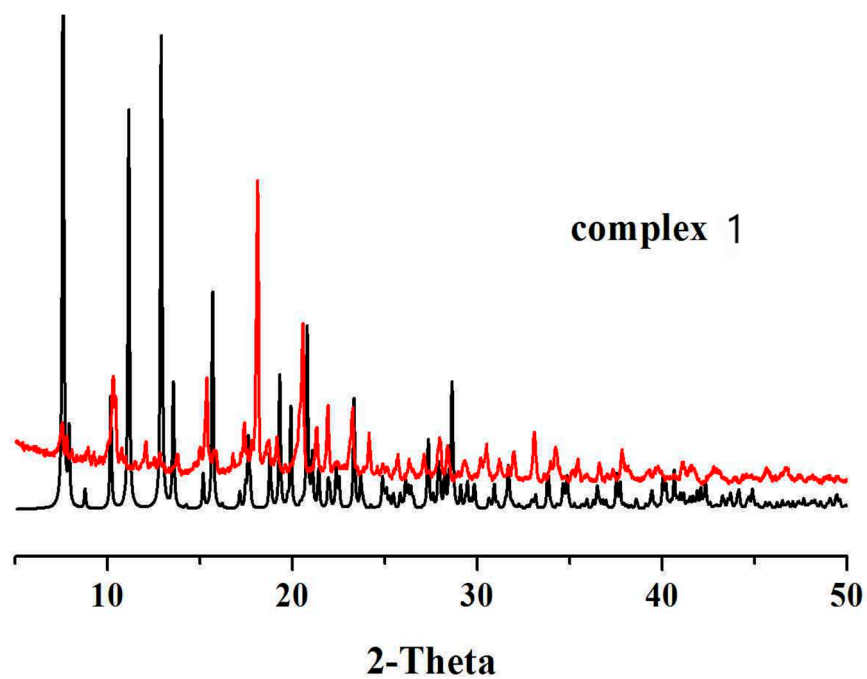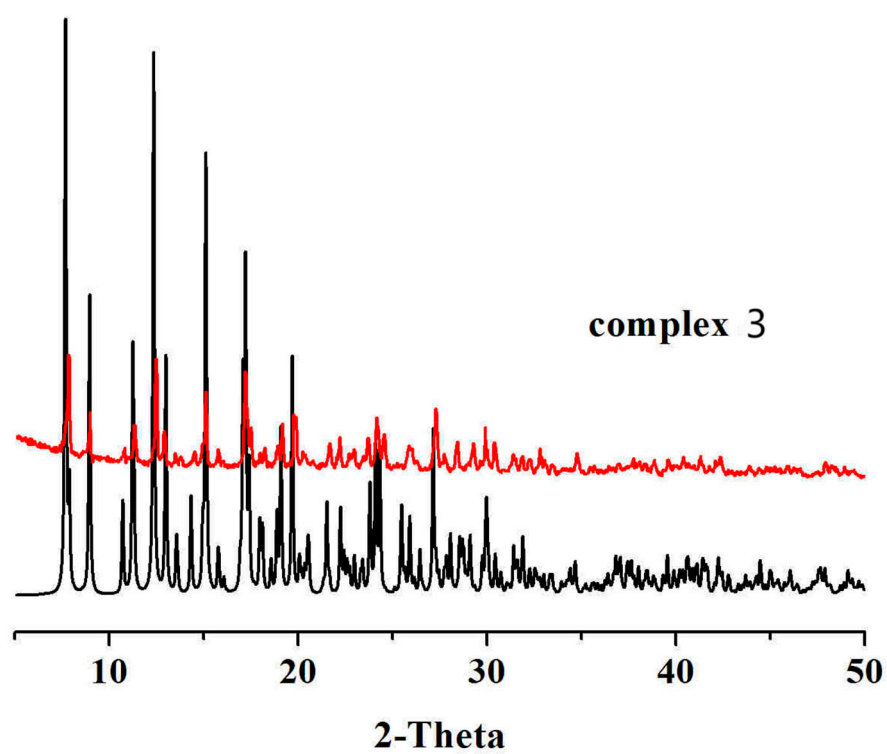

Figure S1. The 3D framework of complex **3**.

Figure S2. Experimental (red) and simulated (black) PXRD patterns of **1–3**.